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Supplementary Information

A two-dimensional magnetic hybrid material based on intercalation of a cationic prussian blue analogue in montmorillonite nanoclay

Dimitrios Gournis,* Christina Papachristodoulou, Enrico Maccallini, Petra Rudolf,* Michael A. Karakassides, Dimitrios T. Karamanis, Marie-Hélène Sage, Thomas T.M. Palstra, Jean-François Colomer, Konstantinos D. Papavasileiou, Vasilios S. Melissas and Nicolaos H. Gangas*

Cartesian coordinates of the optimised Al-FCC complex structure.

1	Fe	0.000	0.000	0.000
2	Fe	0.000	0.000	-5.000
3	Fe	0.000	5.000	0.000
4	Fe	5.000	0.000	0.000
5	Fe	0.000	5.000	-5.000
6	Fe	5.000	0.000	-5.000
7	Fe	5.000	5.000	0.000
8	Fe	5.000	5.000	-5.000
9	N	0.000	3.074	0.000
10	C	0.000	1.898	0.000
11	N	0.000	0.000	-3.074
12	C	0.000	0.000	-1.898
13	N	0.000	5.000	-1.926
14	C	0.000	5.000	-3.102
15	N	5.000	0.000	-1.926
16	C	5.000	0.000	-3.102
17	N	5.000	5.000	-3.074
18	C	5.000	5.000	-1.898
19	N	1.926	5.000	0.000
20	C	3.102	5.000	0.000
21	N	3.074	5.000	-5.000
22	C	1.898	5.000	-5.000
23	N	1.926	0.000	-5.000
24	C	3.102	0.000	-5.000
25	N	0.000	1.926	-5.000
26	C	0.000	3.102	-5.000
27	N	5.000	3.074	-5.000
28	C	5.000	1.898	-5.000
29	N	5.000	1.926	0.000

30	C	5.000	3.102	0.000
31	Al	3.499	1.656	-1.437
32	N	3.074	0.000	0.000
33	C	1.898	0.000	0.000
34	Al	1.497	6.570	-1.392
35	Al	8.510	3.350	-1.429
36	Al	6.488	8.423	-1.403
37	C	8.102	0.000	0.000
38	C	8.102	5.000	-5.000
39	N	8.074	5.000	0.000
40	N	5.000	8.074	0.000
41	C	0.000	8.102	0.000
42	C	5.000	8.102	-5.000
43	N	5.000	6.926	-5.000
44	N	0.000	8.074	-5.000
45	C	0.000	6.898	-5.000
46	O	5.833	7.494	-2.689
47	H	4.900	7.201	-2.551
48	O	7.060	2.622	-1.853
49	H	6.115	2.695	-2.098
50	O	9.520	2.593	-2.619
51	H	9.059	1.838	-2.999
52	O	8.141	7.894	-1.796
53	H	7.896	7.187	-2.438
54	O	4.531	2.391	-2.615
55	H	4.103	3.154	-2.986
56	O	2.037	2.369	-1.842
57	H	1.092	2.295	-2.089
58	O	0.844	7.485	-2.690
59	H	-0.086	7.775	-2.574
60	O	3.123	7.086	-1.803
61	H	2.911	7.797	-2.453
62	N	6.926	0.000	0.000
63	C	6.898	5.000	0.000
64	N	0.000	6.926	0.000
65	C	5.000	6.898	0.000
66	N	6.926	5.000	-5.000
67	C	6.898	0.000	-5.000
68	N	8.074	0.000	-5.000